

Comment on “Isoelectronic Ru substitution at Fe-site in $\text{Sm}(\text{Fe}_{1-x}\text{Ru}_x)\text{AsO}_{0.85}\text{F}_{0.15}$ compound and its effects on structural, superconducting and normal state properties” (arXiv:1004.1978)

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Based on the five-orbital model, we derive the reduced impurity scattering rate $g = z\gamma/2\pi T_{c0}$ in $\text{Sm}(\text{Fe}_{1-x}\text{Ru}_x)\text{AsO}_{0.85}\text{F}_{0.15}$ from the residual resistivity. At $x = 0$, the transition temperature is $T_{c0} = 50$ K. For $0.05 \leq x \leq 0.36$ ($0.84 \geq T_c/T_{c0} \geq 0.3$) the obtained value of g ranges from 1.5 to 2.9, which suggests that the s_{\pm} -wave state cannot survive. We point out that the magnetoresistance frequently gives an underestimated value of g in correlated electron systems.

In Ref. [1], it was shown that the transition temperature in polycrystal $\text{Sm}(\text{Fe}_{1-x}\text{Ru}_x)\text{AsO}_{0.85}\text{F}_{0.15}$ at $x = 0$, $T_{c0} = 50$ K, decreases to $T_c = 15$ K at $x = 0.36$, and $T_c = 0$ K at $x = 0.75$. The observed weak x -dependence of T_c is consistent with previous reports [2, 3]. The authors discussed the reduced scattering rate $g = z\gamma/2\pi T_{c0}$ where γ is the electron scattering rate and $z = m/m^*$ is the renormalization factor. Theoretically, the sign reversal s -wave (s_{\pm} -wave) state vanishes for $g > g_c^{s_{\pm}} = 0.23$ [4]; $g_c^{s_{\pm}} \ll 1$ due to large interband impurity scattering, since all bands are composed of the same d -orbitals. Thus, it is essential to derive g from experiments.

Here, we derive a reliable value of g from the the residual resistivity ρ_0 , since we can calculate ρ_0 with enough accuracy due to the fact that the realistic five-orbital model is available [5]. In the linear-response theory, $\sigma_{xx} = \frac{e^2}{4\pi c} \sum_i \int_{\text{FS}_i} dS_{\mathbf{k}} \frac{|\mathbf{v}_{\mathbf{k}}^i|^2}{2\gamma}$ [4], where i represents the Fermi surfaces, $\mathbf{v}_{\mathbf{k}}^i = \nabla_{\mathbf{k}} E_{\mathbf{k}}^i$, and c is the inter-layer spacing. Using the five-orbital model, we obtain the relation $\rho[\mu\Omega\text{cm}] = 0.24\gamma[\text{K}]$ in 1111 systems ($c = 0.8\text{nm}$) for the filling $n = 5.8 - 6.1$. Then, g is given as $g = 0.66z \cdot \rho_0[\mu\Omega\text{cm}]/T_{c0}[\text{K}]$. In the derivation, correct physical quantities, such as carrier density and Fermi velocity, are maintained automatically. In the *single crystal* $\text{NdFeAsO}_{0.7}\text{F}_{0.3}$ with $T_{c0} = 46.4$ K, T_c decreases to $T_{c0}/2$ by α -particle irradiation when $\rho_0 \sim 480 \mu\Omega\text{cm}$. Thus, T_c is halved when $g = 3.4 = 15g_c^{s_{\pm}}$ for $z = 1/2$.

Next, we discuss $\text{Sm}(\text{Fe}_{1-x}\text{Ru}_x)\text{AsO}_{0.85}\text{F}_{0.15}$. According to Fig. 15 of Ref. [1], $\rho_0^{\text{poly}} \sim 900 \mu\Omega\text{cm}$ at $x = 0.05$ ($T_c = 42\text{K}$), which corresponds to $\rho_0^{\text{single}} \sim 220 \mu\Omega\text{cm}$ in the single crystal, if we apply the empirical relation $\rho^{\text{poly}}/\rho^{\text{single}} \sim 4$ [2]. Since the corresponding g is 1.5 for $z = 1/2$, s_{\pm} -wave state cannot survive against 5% Ru impurities, unless $\rho^{\text{poly}}/\rho^{\text{single}} > 26$. These results are consistent with the previous report for Nd1111 [2]. We also obtain $g \sim 2.9$ at $x = 0.36$ ($T_c = 15$ K) where $\rho_0^{\text{poly}} \sim 1750 \mu\Omega\text{cm}$. However, the reduced scattering rates derived from the magnetoresistance $\Delta\rho/\rho_0 \equiv (\mu_{\text{MR}}B)^2$ and Hall angle $\sigma_{xy}/\sigma_{xx} \equiv \mu_{\text{H}}B$ at $x = 0.36$ in Ref. [1] are $g_{\text{MR}} \sim 0.5$ and $g_{\text{H}} \sim 7.5$ at 57K, respectively [6]. For $0.05 \leq x \leq 0.33$, $g_{\text{MR}} = 0.9 - 1.5$ and $g_{\text{H}} = 1.1 - 7.5$

according to Fig. 12 of Ref. [1]. Thus, both g_{MR} and g_{H} exceed $g_c^{s_{\pm}}$ for $x \geq 0.05$.

It should be noticed that $\mu_{\text{H,MR}}$ can prominently deviate from the true mobility in correlated metals. For example, the ratio $r \equiv \mu_{\text{MR}}/\mu_{\text{H}}$ is not unity in general. The inset of Fig. 3(b) in Ref. [7] shows that the relation $\Delta\rho/\rho_0/(\sigma_{xy}/\sigma_{xx})^2 = r^2 \approx 9$ holds in single crystal $\text{BaFe}_2(\text{As,P})_2$, suggesting that $r \approx 3$. In high- T_c cuprates, $r^2 \sim 3$ in Y- and Bi-based compounds, whereas $r^2 \approx 14$ in $\text{La}_{1-x}\text{Sr}_x\text{CuO}_4$ at $x = 0.17$ [8], and $r^2 \sim 100$ at $x \gtrsim 0.23$ [9]. Thus, the material dependence of $r = \mu_{\text{MR}}/\mu_{\text{H}}$ is very large even in systems with single Fermi surface [11]. [For example, r becomes large when mean-free-path is anisotropic [10].] Moreover, $\mu_{\text{H,MR}}$ can deviate from the true mobility below ~ 200 K due to the current vertex correction (CVC) in the presence of strong spin (or orbital) fluctuations [11]. In fact, Ref. [7] revealed the significant role of the CVC in $\text{BaFe}_2(\text{As,P})_2$.

To summarize, we derived the expression $g = 0.66z \cdot \rho_0^{\text{single}}[\mu\Omega\text{cm}]/T_{c0}[\text{K}]$, which is reliable since ρ_0/γ essentially depends only on the averaged k_{F} and v_{F} for each Fermi surface, whereas insensitive to the correlation effects. For the s_{\pm} -wave state, the critical residual resistivity for $g_c^{s_{\pm}} = 0.23$ is only $35 \mu\Omega\text{cm}$ if $z \sim 1/2$. This fact supports the s_{++} -wave state predicted by the orbital-fluctuation theory [12]. Slow decrease in T_c ($-\Delta T_c \sim 2\text{K}$ per 1% impurities) might originate from the localization effect or reduction of orbital fluctuations by impurities. In contrast to ρ_0 , Hall angle and $\Delta\rho/\rho_0$ are not simply scaled by γ since they are sensitive to other factors, like the Fermi velocity anisotropy and the CVC. Therefore, we have to take care in deriving g from them.

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$T = 200$ K, at which the CVC would be small.

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magneto-conductivity are respectively given by $\sigma_{xy} \sim B \sum_i \langle |\mathbf{l}_{\mathbf{k}}|^2 (\partial\theta_{\mathbf{k}}/\partial k_{\parallel}) \rangle_{\text{FS}i}$ and $\Delta\sigma_{xx} \sim -B^2 \sum_i \langle (l_{\mathbf{k}}^2 (\partial\theta_{\mathbf{k}}/\partial k_{\parallel})^2 \gamma_{\mathbf{k}}^{-1} + (\partial|\mathbf{l}_{\mathbf{k}}|/\partial k_{\parallel})^2 \gamma_{\mathbf{k}}^{-1}) \rangle_{\text{FS}i}$, where $\mathbf{l}_{\mathbf{k}}$ is the mean-free-path including the CVC, and $\theta_{\mathbf{k}} = \tan^{-1}(l_{\mathbf{k}x}/l_{\mathbf{k}y})$. Note that $\Delta\rho/\rho_0 = -\Delta\sigma_{xx}/\sigma_{xx} - (\sigma_{xy}/\sigma_{xx})^2$. Since the CVC enlarge $\partial\theta_{\mathbf{k}}/\partial k_{\parallel}$ near the cold-spot, both R_{H} and $\Delta\rho/\rho_0$ are enhanced near quantum-critical-points. In addition, $\Delta\rho/\rho_0$ becomes large when $\mathbf{l}_{\mathbf{k}}$ is anisotropic due to the second term in $\Delta\sigma_{xx}$.

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